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Pitch-Angle Diffusion in Canonical Coordinates: A Theoretical Formulation

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The equation for pitch-angle diffusion (at constant particle energy E and shell parameter L) in a dipole field can be transformed into canonical form, namely $\partial \bar{f}/\partial t = (\partial/\partial z)[D_{zz}(\partial \bar{f}/\partial z)]$, by the introduction of a new coordinate called z. The new coordinate is obtained by integrating the bounce period of a particle (at fixed E and L) with respect to y^2, where y is the sine of the equatorial pitch angle α_0. A potpourri of applications serves to illustrate the usefulness of such a transformation. For example, if D_{zz} is a suitably simple function of z, one can specify the eigenfunctions $g_n(z)$ of

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the diffusion operator is closed form. If D_{zz} differs only slightly from such a simple function of z, then the corresponding eigenfunctions can be generated from the above set by procedures analogous to the Rayleigh-Schrödinger perturbation theory used in quantum mechanics. The availability of such eigenfunctions enables one to evaluate quantitatively the manner in which geomagnetically trapped particles are redistributed in α_0 and lost from the magnetosphere as the phase-space density $\bar{f}$ evolves in time.

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PREFACE

The author thanks Dr. G. A. Paulikas for his comments on preliminary drafts of the manuscript and Dr. John M. Cornwall *for his suggestion that a variational principle be identified.*

CONTENTS

FIGURE

INTRODUCTION

It is a well-known result in magnetospheric physics that the phase-space density $\bar{f}$ (averaged over gyration, bounce, and drift) evolves according to the equation

$$\frac{\partial \bar{f}}{\partial t} = \frac{1}{x\,T(y)} \frac{\partial}{\partial x}\left[x T(y)\, D_{xx} \frac{\partial \bar{f}}{\partial x}\right] + \bar{S} \qquad (1)$$

in the presence of (a) pitch-angle diffusion at fixed particle energy E and shell parameter L and (b) a distributed source $\bar{S}$ (MacDonald and Walt, 1961; Haerendel, 1968; Roberts, 1969; Walt, 1970; Lyons et al., 1972; Schulz and Lanzerotti, 1974). The diffusion coordinate x is the cosine of the equatorial pitch angle α_0 in this formulation, and the factor T(y) is well approximated (Davidson, 1976) by the formula

$$T(y) \approx T(0) - [T(0) - T(1)]\, y^{3/4}, \qquad (2)$$

where $T(0) \approx 1.3801730$, $T(1) = (\pi/6)(2)^{1/2} \approx 0.7404805$, and $y \equiv \sin \alpha_0 \equiv (1 - x^2)^{1/2}$. Eigenfunction solutions of (1) have been obtained by MacDonald and Walt (1961) and by Roberts (1969) for particular functional forms of the bounce-averaged diffusion coefficient D_{xx} under the approximation that T(y) commutes with $\partial/\partial x$. The difficulty with such an approximation is that it is credible only for $x^2 \ll 1$, whereas one often requires solutions that are valid over the entire interval $0 \le x^2 \le 1$.

The purpose of the present work is to introduce a new diffusion coordinate called z, in terms of which (1) can be solved without further approximation over the entire range of x for selected forms of $D_{zz} \equiv [xT(y)]^2 D_{xx}$. The new coordinate is defined by the equation

$$z = Z(y) \equiv \int_0^x x' T(y') \, dx' = \int_y^1 y' \; T(y') \, dy'$$

$$\approx \frac{1}{2}(1 - y^2) T(0) - \frac{4}{11}\left[T(0) - T(1)\right](1 - y^{11/4}) \qquad (3)$$

and can be shown (Schulz, 1974) to assume the end-point values Z(0) = 16/35 and Z(1) = 0 exactly. The approximation for Z(0) extracted from (3) agrees with 16/35 to within 0.1% (Schulz, 1976). It follows from (1) and (3) that

$$\frac{\partial \bar{f}}{\partial t} = \frac{\partial}{\partial z}\left[D_{zz} \frac{\partial \bar{f}}{\partial z}\right] + \bar{S} \qquad (4)$$

with D_{zz} defined as above. This last form of the diffusion equation is canonical in the sense that there is no intervening Jacobian factor that fails to commute with $\partial/\partial z$. Thus, if D_{zz} is a suitably simple function of z, then one can specify the eigenfunctions $g_n(z)$ of the diffusion operator in closed form by requiring $g_n(z_c)$ to vanish for some positive $z_c < 16/35$. The resulting eigenfunctions will be applicable to the entire physical range $(0 \le z \le z_c < 16/35)$ of the new canonical diffusion coordinate z.

If D_{zz} is not precisely of such a form that yields $g_n(z)$ in terms of previously studied analytical functions, it may nevertheless happen that D_{zz} closely resembles in form a diffusion coefficient $\bar{D}_{zz}$ for which the eigenfunctions $\bar{g}_n(z)$ are known exactly. In this case one may be able to use the $\bar{g}_n(z)$ as a basis for generating the $g_n(z)$ by means of perturbation theory. These and other applications of the coordinate z are examined below.

EXACT EIGENFUNCTIONS

The functional form of D_{zz} is neither well known nor easily (cf. Lyons et al., 1972) derived. However, the construction of pitch-angle eigenfunctions $g_n(z)$ for (4) can be illustrated quantitatively if one arbitrarily assumes that $D_{zz} = (z/z_c)^{\sigma} D_{zz}^*$, where $\sigma < 2$ and D_{zz}^* is the value of D_{zz} at some $z = z_c$ $< 16/35$ where $\bar{f}$ is required to vanish. There is a precedent for this type of exercise in the work of Roberts (1969), who sought solutions of (1) for $D_{xx} = (x/x_c)^{\xi} D_{xx}^*$ under the assumption that T(y) would commute with $\partial/\partial x$. The present form of D_{zz} agrees with the Roberts (1969) form of D_{xx} for $x^2 \ll 1$ if one takes $\xi = 2\sigma - 2$, but both forms are equally arbitrary.

There is a broader purpose behind an exercise of this type. By identifying certain functional forms of D_{zz} for which the eigenfunctions of the diffusion operator can be expressed in closed form, one thereby obtains a complete set of orthogonal functions on the interval $0 \le z \le z_c$. The eigenfunctions corresponding to a somewhat different form of D_{zz} can be expanded in terms of this set, and the expansion coefficients can be determined by means of perturbation theory.

For this purpose, it proves useful (see above) to adopt the notation $\bar{D}_{zz}$ for any special form of D_{zz} that leads to eigenfunctions which can be written explicitly in closed form. It is logical then to denote the eigenvalues of the diffusion operator as $\bar{\lambda}_n$ and the corresponding eigenfunctions as $\bar{g}_n(z)$ when D_{zz} has such a special form. Thus, in the present context, one is considering the special case in which $\bar{D}_{zz} = (z/z_c)^{\sigma}\bar{D}_{zz}^{*}$, where $\sigma < 2$ and $\bar{D}_{zz}^{*}$ is the value of $\bar{D}_{zz}$ at $z = z_c$.

Following the mathematical methods of Roberts (1969), one seeks solutions of the eigenvalue equation

$$(d/dz)\,[\,\bar{D}_{zz}\,(d\bar{g}_n/dz)\,] + \bar{\lambda}_n\bar{g}_n = 0 \tag{5}$$

in the form $\bar{g}_n(z) \propto z^{\alpha}w(\beta z^{\gamma})$ for $\bar{D}_{zz} = (z/z_c)^{\sigma}\bar{D}_{zz}^{*}$. Since (5) then reduces to Bessel's equation for $\gamma = 1 - (\sigma/2)$, $\alpha = (1-\sigma)/2$, and $\beta^2 = \bar{\lambda}_n z_c^{\sigma}/\bar{D}_{zz}^{*}\gamma^2$, it follows that the eigenfunctions of (5) are given by

$$\bar{g}_n(z) = [\,(2-\sigma)/z_c\,]^{1/2}\,[\,J_{\nu}'(\kappa_{\nu n})\,]^{-1}$$

$$\times\,(z/z_c)^{(1-\sigma)/2}\,J_{\nu}(\kappa_{\nu n}(z/z_c)^{1-(\sigma/2)}), \tag{6}$$

where $\kappa_{\nu n}$ (n = 0, 1, 2, . . .) is the nth zero of the ordinary Bessel function of order $\nu = (\sigma - 1)/(2 - \sigma)$, i.e., where $J_\nu(\kappa_{\nu n}) = 0$. The corresponding eigenvalue is given by

$$\bar{\lambda}_n = (\kappa_{\nu n} / 2 z_c)^2 (2 - \sigma)^2 \bar{D}_{zz}^*, \tag{7}$$

and the normalization of (6) has been chosen so that

$$\int_0^{z_c} \bar{g}_n(z)\, \bar{g}_m(z)\, dz = \delta_{nm} \equiv \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases} \tag{8}$$

Sinze z is given by (3) as a function of $y \equiv (1 - x^2)^{1/2}$, it is easy enough to plot $\bar{g}_n(z)$ as a function of the more familiar variable x. However, no immediate purpose would be served by such a plot, since the form of $\bar{D}_{zz}$ leading to (6) and (7) does not correspond exactly to the functional form of D_{xx} postulated by Roberts (1969) except in the limit $x \to 0$; nor does it correspond to the functional form of D_{xx} used by anyone else. Therefore, illustration of the functional form of $\bar{g}_n(z)$ is deferred for now and is given instead in the accompanying numerical-applications paper by Schulz and Boucher (1981), wherein the eigenfunctions corresponding to $D_{xx} = (x/x_c)^{\xi} D_{xx}^*$ are estimated successively for comparison with the results of Roberts (1969).

The form $\bar{D}_{zz} = (z/z_c)^{\sigma} \bar{D}_{zz}^*$ considered above is not the only form of $\bar{D}_{zz}$ that yields exact expressions for the eigenfunctions of (5). Another form of $\bar{D}_{zz}$ that leads to exact eigenfunctions is the form

$\bar{D}_{zz} = (1 - \alpha^2 z^2)\,\bar{D}_{zz}^{\,0}$, where $0 < \alpha z_c < 1$ and $\bar{D}_{zz}^{\,0}$ denotes the value of $\bar{D}_{zz}$ at $z = 0$. This form of $\bar{D}_{zz}$ converts (5) into Legendre's equation in the variable $\zeta \equiv \alpha z$. Solutions are given in unnormalized form by the expression

$$\bar{g}_\nu(z) \propto Q_\nu(\alpha z_c)\, P_\nu(\alpha z) - P_\nu(\alpha z_c)\, Q_\nu(\alpha z), \tag{9}$$

where $P_\nu(\zeta)$ and $Q_\nu(\zeta)$ are the two kinds of Legendre function of degree ν and order $\mu = 0$ (Stegun, 1966). The corresponding eigenvalues $\bar{\lambda}_\nu$ are given by

$$\bar{\lambda}_\nu = \alpha^2 \nu(\nu + 1)\, D_{zz}^{\,0}. \tag{10}$$

Acceptable values of $\nu\,(> 0)$ are restricted by the condition

$$R_\nu(\alpha z_c) \equiv \cos(\nu\pi/2)\, P_\nu(\alpha z_c) - (2/\pi)\sin(\nu\pi/2)\, Q_\nu(\alpha z_c) = 0, \tag{11}$$

which assures that $\lim \left[\bar{D}_{zz}\, \bar{g}_\nu'(z)\right] = 0$ as $z \to 0$. The significance of this latter requirement is that there must be no diffusion current across the "boundary" at $z = 0$, since particles cannot be lost by having their mirror points reach the equator. The eigenfunctions $\bar{g}_\nu(z)$ and $\bar{g}_\rho(z)$ corresponding to distinct eigenvalues $\bar{\lambda}_\nu$ and $\bar{\lambda}_\rho$ are orthogonal in the sense of (8), but calculation of the appropriate normalization constant for (9) in closed form appears to be intractable.

The case $\alpha = 0$ is not included in (9)-(11). Eigenfunctions in this case are given by

$$\bar{g}_n(z) = (2/z_c)^{1/2} \cos [(2n + 1)(\pi z/2z_c)], \tag{12}$$

and the corresponding eigenvalues are given by

$$\bar{\lambda}_n = (2n + 1)^2 (\pi/2z_c)^2 \bar{D}_{zz}^0 \tag{13}$$

for $n = 0, 1, 2, \ldots$; this case is also covered by (5)-(8) with $\sigma = 0$ ($\nu = -1/2$), since one knows (e.g., Antosiewicz, 1966) that $J_{-1/2}(\zeta) = (2/\pi\zeta)^{1/2} \times \cos\zeta$. Moreover, one finds $\bar{D}_{zz}^* = \bar{D}_{zz}^0$ by definition for $\sigma = 0$.

The distribution of eigenvalues is immediately apparent from (13) for the case in which $\bar{D}_{zz}$ is independent of z. However, the explicit forms of $\kappa_{\nu n}$ in (7) and of ν in (10) are available only in the asymptotic ($n \rightarrow \infty$) limit if $\bar{D}_{zz}$ varies with z. Asymptotic expansion of $J_\nu(\kappa_{\nu n}) = 0$ in (6) for large argument yields

$$J_\nu(\kappa_{\nu n}) \sim (2/\pi\kappa_{\nu n})^{1/2} \cos[\kappa_{\nu n} - \nu(\pi/2) - (\pi/4)], \tag{14}$$

which is to say that

$$\kappa_{\nu n} \sim n\pi + [(4 - \sigma)/(2 - \sigma)](\pi/4). \tag{15}$$

The asymptotic expansion of $\kappa_{\nu n}$ given by (15) yields all the eigenvalues exactly for $\sigma = 0$ [see (13)] but is only indicative for other values of $\sigma < 2$. On the other hand, the asymptotic expansion of $R_\nu(\alpha z_c) = 0$ in (11) for large ν yields

$$R_\nu(\alpha z_c) \sim (2/\pi\nu \sin\theta)^{1/2} \cos\{ [\nu + (1/2)] [\theta - (\pi/2)] \} = 0, \tag{16}$$

where $\theta \equiv \cos^{-1}(\alpha z_c)$. This means that

$$\nu \sim [(2n+1)\pi/(\pi - 2\theta)] - (1/2) \tag{17}$$

for large integers n. If one substitutes (17) in (10) and takes the limit $\alpha \to 0$, the eigenvalues λ_ν approach those given by (13) for the corresponding values of n.

PERTURBATION THEORY

It would be fortuitous if the form of D_{zz} in a realistic situation corresponded exactly to an idealized form ($\bar{D}_{zz}$) known to yield eigenfunctions in closed form. However, it is not unreasonable to expect that the physically realistic D_{zz} might be roughly approximated by some such $\bar{D}_{zz}$.

In this case one might be able to use the eigenfunctions $\overline{g}_n(z)$ that correspond to $\overline{D}_{zz}$ as a basis (i.e., as a complete set of orthogonal functions) for generating by means of perturbation theory the eigenfunctions $g_n(z)$ that correspond to D_{zz}.

Let the linear transformation between the true eigenfunctions $g_n(z)$ and the basis functions $\overline{g}_n(z)$ be specified by

$$g_n(z) = \sum_{m=0}^{\infty} \overline{g}_m(z)\, U_{mn}, \tag{18}$$

where the expansion coefficients U_{mn} form a real unitary matrix, i.e., a matrix such that

$$\sum_{m=0}^{\infty} U_{mp}\, U_{mn} = \delta_{pn}. \tag{19}$$

The expansion coefficients U_{mn} are otherwise unknown at this stage. However, the contention that $g_n(z)$ is an eigenfunction corresponding to D_{zz} must mean that

$$(d/dz)\, [D_{zz}(dg_n/dz)\,] + \lambda_n g_n = 0 \tag{20}$$

for some λ_n [compare with (5)]. By invoking the orthogonality property specified by (8), one thereby derives from (18) and (20) the condition

$$\sum_{m=0}^{\infty} (\Lambda_{pm} - \lambda_n \delta_{pm}) U_{mn} = 0 \tag{21}$$

on the expansion coefficients U_{mn}, where

$$\Lambda_{pm} \equiv -\int_0^{z_c} \bar{g}_p \,(d/dz)\left[\bar{D}_{zz}(d\bar{g}_m/dz)\right] \, dz$$

$$= \int_0^{z_c} (d\bar{g}_p/dz)\, D_{zz}\, (d\bar{g}_m/dz)\, dz. \tag{22}$$

The second (i. e., the manifestly symmetric) integral expression for Λ_{pm} is derived from the first through integration by parts. One makes use here of the fact that $\bar{g}_p(z_c) = 0$ and the requirement (compare above) that $\lim\, [D_{zz}\, \bar{g}_m'(z)\,] = 0$ as $z \to 0$. This latter requirement means that one must select $\bar{D}_{zz}$ so that $\lim\, (\bar{D}_{zz}/D_{zz}) \neq 0$ as $z \to 0$, i.e., so that the $\bar{g}_m(z)$ do not transport particles across the kinematical "boundary" at $z = 0$.

It follows from (21) that the columns of the unitary matrix U_{mn} are the normalized eigenvectors of the real symmetric matrix Λ_{pm}, and that the λ_n are the corresponding eigenvalues. Thus, the problem of identifying the eigenfunctions and eigenvalues of (20) has been reduced to the problem of diagonalizing the matrix Λ_{pm} specified by (22). One observes from the first integral expression for Λ_{pm} that if $\bar{D}_{zz} \equiv D_{zz}$, then $\Lambda_{pm} = \delta_{pm}\, \lambda_m$. This follows from (5) and (8). Consequently, if $\bar{D}_{zz}$ is a reasonably good approximation of D_{zz}, then the off-diagonal elements of Λ_{pm} will be "small" in the sense required by perturbation theory.

The usual procedure for diagonalizing a matrix such as Λ_{pm} is to seek (eigenvalue) solutions λ_n of the characteristic equation

$$\det(\Lambda_{pm} - \delta_{pm}\lambda) = 0. \tag{23}$$

When one seeks to expand the above determinant by minors, it becomes obvious that factors lying off the main diagonal can affect λ_n only to second or higher order. Thus, if terms of second and higher order are neglected, one obtains

$$\lambda_n \approx \Lambda_{nn} = \bar{\lambda}_n + \int_0^{z_c} (D_{zz} - \bar{D}_{zz})\,(d\bar{g}_n/dz)^2\,dz \tag{24}$$

for the eigenvalues and

$$U_{kn}/U_{nn} \approx \Lambda_{kn}/(\Lambda_{nn} - \Lambda_{kk}), \qquad k \neq n \tag{25}$$

for the components of the corresponding eigenvectors. One can normalize (25) in accordance with (19) by setting

$$U_{nn} \approx \left\{1 + \sum_{k\neq n}[\Lambda_{kn}/(\Lambda_{nn} - \Lambda_{kk})]^2\right\}^{-1/2} \tag{26}$$

although it is apparent from (26) that $U_{nn} \approx 1$ except for corrections of second or higher order in "small" quantities.

The foregoing results actually represent somewhat of an improvement (cf. Morse and Feshbach, 1953) over those obtained by the usual Rayleigh-Schrödinger method encountered in quantum mechanics (e.g., Schiff, 1955). The advantage of the present method over Rayleigh-Schrödinger is that the denominator in (25) contains a better approximation to the difference between the true eigenvalues. The author has been informed by Cornwall (1977) that the present perturbation method is known in quantum mechanics as the Wigner-Brillouin method. Expanding (23) to second order in off-diagonal elements, one readily obtains

$$\lambda_n \approx \Lambda_{nn} - \sum_{k \neq n} \frac{\Lambda_{kn}\Lambda_{nk}}{\Lambda_{kk} - \Lambda_{nn}} \tag{27}$$

as an improvement on the second-order Rayleigh-Schrödinger result for non-degenerate states, which the diffusion eigenfunctions clearly are. Substitution of (27) in (21) yields a general equation of the form

$$\left[\Lambda_{kk} - \Lambda_{nn} + \sum_{j \neq n} \frac{\Lambda_{nj}\Lambda_{jn}}{\Lambda_{jj} - \Lambda_{nn}}\right]\frac{U_{kn}}{U_{nn}} + \Lambda_{kn} + \sum_{j \neq k,n} \Lambda_{kj}(U_{jn}/U_{nn}) \approx 0 \tag{28}$$

for calculating the second-order eigenvectors. Since Λ_{kj} and U_{jn} are both "small" quantities for $k \neq j \neq n$, it will be sufficient (for the second-order accuracy of the off-diagonal elements U_{kn}) to estimate the ratios U_{jn}/U_{nn} in (28) by means of (25). Similarly, one can neglect the summation that appears in the square-bracketed coefficient of U_{kn}/U_{nn} in (28) without sacrificing the desired order of accuracy. Thus, it follows from (28) that

$$\frac{U_{kn}}{U_{nn}} \approx \frac{1}{\Lambda_{nn} - \Lambda_{kk}}\left[\Lambda_{kn} + \sum_{j \neq k,n} \frac{\Lambda_{kj}\Lambda_{jn}}{\Lambda_{nn} - \Lambda_{jj}}\right] \tag{29}$$

for $k \neq n$. The diagonal elements U_{nn} are to be determined from (19). A first-order expansion of (26) assures unit normalization to second order in "small" quantities. However, the use of (29) in (19) might be preferable, in that this procedure would assure unit normalization of each perturbed eigenvector to all orders.

WKB APPROXIMATION

An alternative construction of eigenfunctions for the case in which D_{zz} varies only weakly with z is familiar from the literature of quantum mechanics. This is the method of Wentzel (1926), Kramers (1926), and Brillouin (1926). The WKB approximation is motivated by transforming (20) into the time-independent Schrödinger equation

$$(d^2 g_n / d\zeta^2) + k^2 g_n = 0. \tag{30}$$

This is achieved by introducing the new variable

$$\zeta = \int_0^z (D_{zz}^* / D_{z'z'}) \, dz', \tag{31}$$

whereupon one obtains

$$k^2 = \lambda_n (D_{zz}^*)^{-2} D_{zz}. \tag{32}$$

Indeed, equations (30)-(32) are valid even for an arbitrary variation of D_{zz} with z. However, if D_{zz} varies only weakly with z, then k must vary only weakly with ζ. In this case one obtains

$$\hat{g}_n(z) \approx D_{zz}^{-1/4}\left[\cos\int_0^z (\lambda_n/D_{z'z'})^{1/2}\,dz'\right]$$

$$\div\left\{\int_0^{z_c} D_{zz}^{-1/2}\left[\cos^2\int_0^z (\lambda_n/D_{z'z'})^{1/2}\,dz'\right]dz\right\}^{1/2} \tag{33}$$

as the WKB solution (e.g., Merzbacher, 1961). The corresponding eigenvalues, determined by requiring that $\hat{g}_n(z_c) = 0$, are given by

$$\hat{\lambda}_n \approx (2n+1)^2 (\pi/2)^2 D_{zz}^* \left[\int_0^{z_c} (D_{zz}^*/D_{zz})^{1/2}\,dz\right]^{-2} \tag{34}$$

The above results for $\hat{g}_n(z)$ and $\hat{\lambda}_n$ reduce (as required) to (12) and (13), respectively, in case D_{zz} is a true constant (altogether independent of z). They provide a viable alternative to perturbation theory (based on the above-described case $\sigma = 0$) if D_{zz} varies weakly with z.

VARIATIONAL PRINCIPLE

A further point deserves consideration, namely that the diagonalization of Λ_{pm} in (21) is equivalent to the implementation of a variational principle (Cornwall, 1977) based on (22). The variational principle asserts that

$$\lambda_0 = \text{Min} \int_0^{z_c} (dg/dz)^2 \, D_{zz} \, dz \tag{35}$$

subject to the constraint that

$$\int_0^{z_c} [g(z)]^2 \, dz = 1, \tag{36}$$

the condition that $\lim [D_{zz} \, g'(z)] = 0$ as $z \to 0$, and the boundary condition that $g(z_c) = 0$.

<u>Proof:</u> Since the eigenfunctions $g_n(z)$ of the true diffusion operator $(d/dz)[D_{zz}(d/dz)]$ form a complete set of orthogonal functions, one can expand any continuous $g(z)$ satisfying (36) so that

$$g(z) = \sum_{n=0}^{\infty} v_n \, g_n(z), \tag{37}$$

where

$$v_0^2 = 1 - \sum_{n=1}^{\infty} v_n^2. \tag{38}$$

The minimization specified by (35) is implemented by varying the (real) expansion coefficients V_n. It follows from (22), (37), and (38) that

$$\int_0^{z_c} (dg/dz)^2 D_{zz} \, dz = \lambda_0 + \sum_{n=1}^{\infty} (\lambda_n - \lambda_0) V_n^2. \quad (39)$$

Since $\lambda_n > \lambda_0$ for $n \geq 1$, i.e., since one of the eigenvalues in (20) must be the smallest, the integral that appears in (35) and (39) can be minimized only by setting $V_n = 0$ for $n \geq 1$. Thus, the integral in (35) and (39) can be minimized only by taking $g(z) = g_0(z)$, in which case the integral becomes equal to λ_0. This is the standard proof (e.g., Schiff, 1955) for the validity of a variational principle.

The usual means of implementing (35) is to construct a trial function $g(z;\alpha_m)$ that meets the required constraints and depends on several adjustable parameters α_m. The integral that appears in (35) is then minimized by varying the adjustable parameters. It is not always practical to obtain eigenfunctions higher than $g_0(z)$ by variational means. One theoretically can do so, as in quantum mechanics (e.g., Merzbacher, 1961), by selecting trial functions that are orthogonal [in the sense of (8)] to the optimal $g_0(z)$ obtained in the manner described immediately above. Such a procedure is often too cumbersome for practical use, especially if the adjustable parameters α_{mn} appear nonlinearly in the specification of the trial functions $g_n(z; \alpha_{mn})$. However, a special case of the variational method is realized if one specifies each $g_n(z; \alpha_{mn})$ as a linear superposition of orthogonal functions $\bar{g}_m(z)$, as in (18). In this case the α_{mn} correspond to the expansion coefficients U_{mn} in (18), and minimization of λ in (35) is equivalent to diagonalization of the matrix Λ_{pm}, as in (21). Of course, the matrices Λ_{pm} and U_{mn} in (21) are of infinite dimension. This precludes their numerical evaluation in complete form. However, progressively better variational approximations of the eigenfunctions $g_n(z)$ can be obtained by diagonalizing progressively larger finite submatrices of Λ_{pm}, i.e., by truncating the summation in (21) at $m = N-1$ for progressively larger values of N.

STEADY STATE

If the phase-averaged source $\overline{S}$ in (4) were constant in time, then the solution $\overline{f}(z, t)$ would approach a steady-state solution $\overline{f}_\infty(z)$ in the limit $t \rightarrow \infty$. Following Roberts (1969), one can obtain this $\overline{f}_\infty(z)$ by integrating (4) twice with respect to z for $\partial\overline{f}/\partial t = 0$. The result

$$\overline{f}_\infty(z) = \int_z^{z_c} (D_{z'z'})^{-1} \int_0^{z'} \overline{S}(z'')\, dz''\, dz' \qquad (40)$$

is obtained upon application of the relevant boundary conditions.

Roberts (1969) has noted that if $\overline{S}$ is assumed independent of x (i.e., independent of z in the present context), then the functional form of $\overline{f}_\infty$ tends to resemble that of the lowest eigenfunction g_0. This tendency can be made understandable by expanding $\overline{S}$ in (4) as a linear combination of the orthogonal eigenfunctions g_n. One thereby obtains

$$\overline{f}_\infty(z) = \sum_{n=0}^{\infty} \lambda_n^{-1}\, g_n(z) \int_0^{z_c} \overline{S}(z')\, g_n(z')\, dz', \qquad (41)$$

where $\overline{S}(z') \geq 0$ by definition (i.e., $\overline{S}$ is a <u>source</u>). As long as $\overline{S}(z')$ in (41) is constant (or at least relatively structureless) over the interval $0 \leq z \leq z_c$, it is likely that the moment of $\overline{S}$ with respect to the positive-definite eigenfunction $g_0(z')$ will exceed those with respect to the oscillatory (not positive-definite) eigenfunctions $g_n(z')$ for $n \geq 1$. This property and the weighting by λ_n^{-1} in (41) would account for the tendency, noted by Roberts (1969), for $\bar{f}_\infty(z)$ to resemble $g_0(z)$ in functional form. Of course, it follows from the completeness of the $g_n(z)$ as an orthonormal set of basis functions that $\bar{f}_\infty$ will coincide exactly with g_0 in functional form only if $\overline{S}$ itself is directly proportional to $g_0(z)$.

OMNIDIRECTIONAL FLUX

It would be appropriate to relate the formal results obtained above to physically observable quantities. Consider an off-equatorial point, i.e., one at which the local magnetic-field intensity B exceeds the equatorial value B_0 on a field line identified by the dimensionless label L. It is well known (e.g., Schulz and Lanzerotti, 1974) that the unidirectional flux of particles (per unit energy and solid angle at local pitch angle α) is equal to $p^2\bar{f}$, with $\bar{f}$ evaluated at

$$y = (B_0/B)^{1/2} \sin \alpha. \tag{42}$$

In order to specify the omnidirectional flux $J_{4\pi}$ (per unit energy) at this point in space, one must integrate $p^2\bar{f}$ over the unit sphere in momentum ($\mathbf{p}$) space. Thus, it follows from (42) that

$$
\begin{aligned}
J_{4\pi} &\equiv 4\pi p^2 \int_0^{\cos\alpha_c} \bar{f}\ d(\cos\alpha) \\
&= 2\pi p^2 \int_{y_c^2}^{B_0/B} (B/B_0)[1 - y^2(B/B_0)]^{-1/2}\ \bar{f}\ d(y^2) \\
&= -2\pi p^2 \int_{y_c^2}^{B_0/B} [1 - y^2(B/B_0)]^{1/2}\ (\partial\bar{f}/\partial z)\ T(y)\ d(y^2) \qquad (43)
\end{aligned}
$$

at $B/B_0 \geq 1$. The final line of (43) results from integration by parts and serves to simplify the required numerical quadrature.

The phase-space density $\bar{f}$ that appears in (43) can be expanded as a weighted series of eigenfunctions of the diffusion operator (Roberts, 1969):

$$
\bar{f} = \bar{f}_\infty(z) + \sum_n A_n(E, L; t)\, g_n(z). \qquad (44)
$$

The omnidirectional flux described by (43) can thus be written in the form

$$
\begin{aligned}
J_{4\pi} = 2\pi p^2 \Big[&(\bar{S}/x_c^2 D_{xx}^*)\, G_\infty(B/B_0) \\
&+ \sum_n A_n(E, L; t)\, G_n(B/B_0) \Big], \qquad (45)
\end{aligned}
$$

where

$$
G_n(B/B_0) = -\int_{y_c^2}^{B_0/B} [1 - y^2(B/B_0)]^{1/2}\, g_n'(z)\ T(y)\ d(y^2) \qquad (46)
$$

and

$$G_\infty(B/B_0) = -(x_c^2 D_{xx}^{*}/\bar{S}) \int_{y_c^2}^{B_0/B} [1 - y^2(B/B_0)]^{1/2} \bar{f}_\infty'(z)\, T(y)\, d(y^2). \tag{47}$$

Another physical quantity of interest is the particle content C (per unit L and energy) of a magnetic drift shell. To obtain this, one must integrate $(1/v) J_{4\pi}$ over the drift-shell volume, where v is the speed of the particle. The cross-sectional area of an infinitesimal drift shell of "width" dL is $2\pi La^2(B_0/B)\,dL$, where a is the radius of the earth. Therefore, the volume per unit "width" is given by

$$\begin{aligned} \frac{dV}{dL} &= 2\pi La^2 \int_0^\pi (B_0/B)\ (ds/d\theta)\, d\theta \\ &= 2\pi L^2 a^3 \int_{-1}^{+1} \sin^6\theta\ d(\cos\theta) = 4\pi(16/35)L^2 a^3, \end{aligned} \tag{48}$$

where θ is the magnetic colatitude and s is the coordinate that measures arc length along the dipolar field line. It follows from the above considerations and from (43) that

$$C = 4\pi^2 La^2 (p^2/v) \int_0^\pi (ds/d\theta) \int_{y_c^2}^{B_0/B} \bar{f} \sec\alpha\, d(y^2)\, d\theta. \tag{49}$$

The integral over y^2 in (49) contains contributions from all particle trajectories that mirror at a higher latitude than the point identified by the local B/B_0. The domain of integration is illustrated in Figure 1. If the order of integration is reversed, then one obtains

$$C = 4\pi^2 L a^2 p^2 \int_{y_c^2}^{1} \bar{f} \int_{-s_m}^{+s_m} (1/v \cos\alpha)\, ds\, d(y^2) \qquad (50)$$

upon recalling that $\bar{f}$ satisfies Liouville's theorem, i.e., that $\bar{f}$ depends on y but not on s. The upper limit s_m in (50) represents the arc length from the equator ($s = 0$) to the mirror point of a particle whose equatorial pitch angle is $\sin^{-1} y$.

The integral of $(1/v \cos\alpha)$ with respect to s in (50) represents half the bounce period of the particle, i.e., is equal to $(2La/v)\, T(y)$, where $T(y)$ is the dimensionless function that appears in (1) and (2). Thus, it follows from (50) that

$$C = 16\pi^2 L^2 a^3 (p^2/v) \int_{y_c}^{1} \bar{f}\; y\, T(y)\, dy$$

$$= 16\pi^2 L^2 a^3 (p^2/v) \int_{0}^{z_c} \bar{f}\, dz. \qquad (51)$$

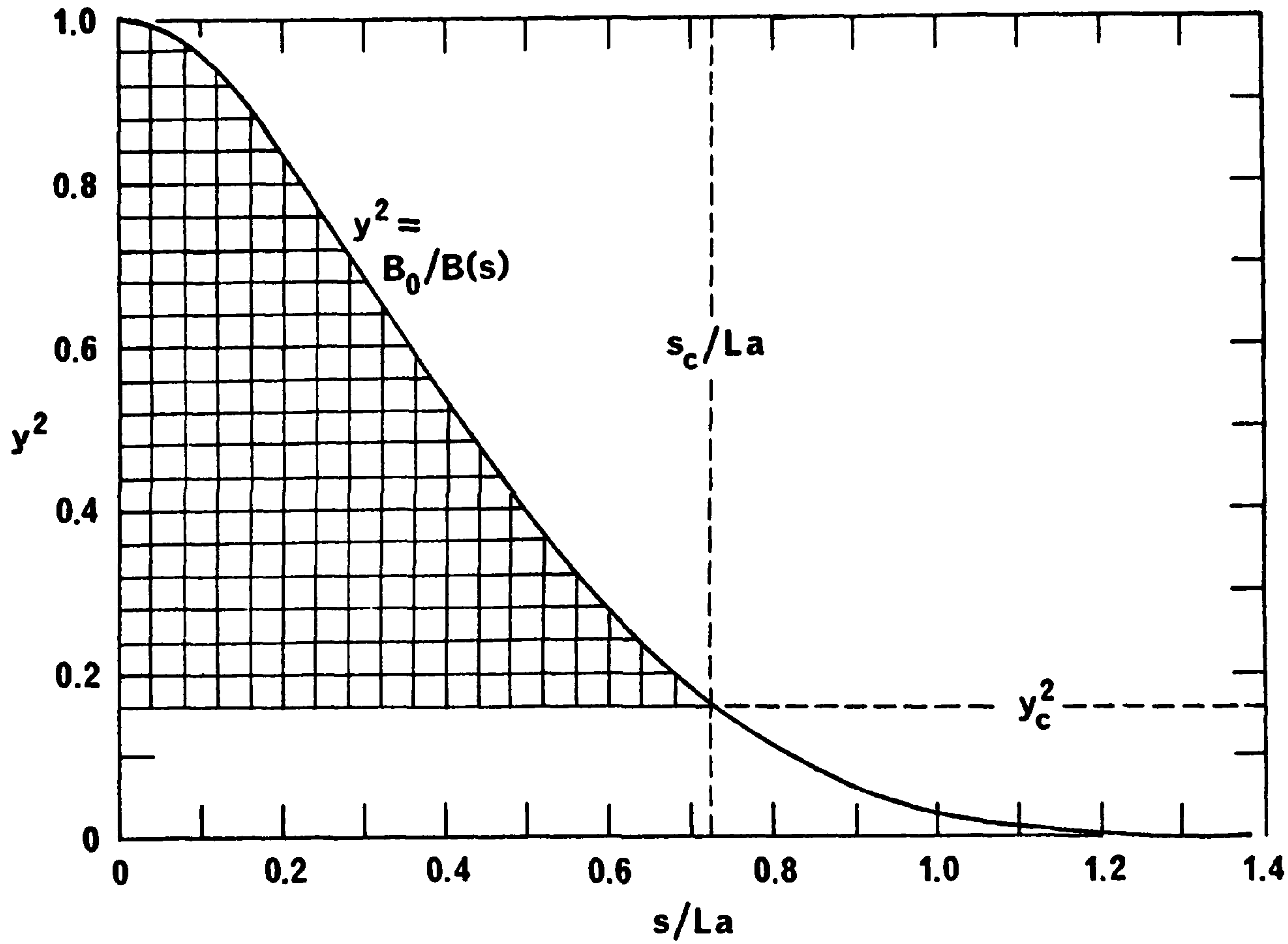

Figure 1. Domain of integration for evaluating particle content of a drift shell, as in (49)-(51).

This relationship brings out the true physical significance of the new diffusion coordinate z, namely that z is a direct measure of phase-space volume at fixed E and L. Such a finding comes as no surprise; if it were not so, then z would not be a canonical coordinate in the sense of (4) and some Jacobian factor would intervene there.

FORMAL CONSIDERATIONS

The canonical coordinate z introduced above is a variable corresponding to the equatorial pitch angle α_0. More generally, one may wish to identify canonical coordinates corresponding (respectively) to kinetic energy E and shell parameter L, so that (in the presence of energy transport and radial diffusion) the Fokker-Planck equation can be written in the canonical form

$$\frac{\partial \bar{f}}{\partial t} = - \sum_{i=1}^{3} \frac{\partial}{\partial Q_i} \left[\left\langle \frac{dQ_i}{dt} \right\rangle \bar{f} \right] + \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial}{\partial Q_i} \left[D_{ij} \frac{\partial \bar{f}}{\partial Q_j} \right] + \bar{S}, \tag{52}$$

where $\langle dQ_i/dt \rangle$ and D_{ij} are the transport coefficients. This will be the case if the new coordinates Q_i are related by a canonical transformation (Goldstein, 1950) to the three adiabatic invariants

$$M = (p^2/2m_0\, B_0)\,(1 - x^2) \qquad (53)$$

$$J = 2\, L\, a\, p\; Y(y) \qquad (54)$$

$$\Phi = (2\pi a^2/L)\,(B_0 L^3)\ \mathrm{sgn}\, q \qquad (55)$$

of charged-particle motion in a dipole field, i.e., if the Jacobian $\partial(M, J, \Phi) / \partial(Q_1, Q_2, Q_3)$ of the transformation from (M, J, Φ) to (Q_1, Q_2, Q_3) is a constant (Haerendel, 1968). The particle described by (53)-(55) has charge q and rest mass m_0. Its scalar momentum is $p = (\gamma^2 - 1)^{1/2} m_0 c$, where $\gamma = 1 + (E/m_0 c^2)$ and c is the speed of light. The particle described by (53)-(55) executes a drift shell, bearing the dimensionless label L, on which the equatorial magnetic field is B_0 (proportional to L^{-3}). The particle has an equatorial pitch angle $\alpha_0 \equiv \sin^{-1} y \equiv \cos^{-1} x$, and the earth has a radius denoted $\underline{a}$. The function $Y(y)$ in (54) is given (Schulz, 1971; Davidson, 1976) by

$$\begin{aligned} Y(y) &= 2y \int_y^1 (y')^{-2}\; T(y')\; dy' \\ &\approx 2\,T(0) + [6\,T(0) - 8\,T(1)]\,y - 8\,[T(0) - T(1)]\,y^{3/4}, \end{aligned} \qquad (56)$$

where $T(y)$, the function specified by (2), is equal to $(p/4\,L\,a\,\gamma\, m_0)$ times the particle's bounce period.

The transformation from (M, J, Φ) to (E, x, L) has a Jacobian that is given by

$$\partial(M, J, \Phi)/\partial(E, x, L) =$$

$$- 8\pi a^2 m_0 c L^2 \gamma(\gamma^2 - 1)^{1/2} \; x \; T(y) \; \mathrm{sgn}\, q. \tag{57}$$

This is therefore not a canonical transformation, since its Jacobian depends on all three of the new kinematic variables: on E through the factor $\gamma(\gamma^2 - 1)^{1/2}$, on x through the factor $x\,T(y)$, and on L through the factor L^2. Making use of this factorization, however, one clearly can construct a set of new variables

$$Q_1 = 3\int_1^{\gamma} [(\gamma')^2 - 1]^{1/2} \gamma' \, d\gamma' = (\gamma^2 - 1)^{3/2} \tag{58}$$

$$Q_2 = \int_0^x x' \, T(y') \, dx' = \int_y^1 y' \, T(y') \, dy' \equiv Z(y) \tag{59}$$

$$Q_3 = 3\int_0^L (L')^2 \, dL' = L^3 \tag{60}$$

such that the Jacobian $\partial(M, J, \Phi)/\partial(Q_1, Q_2, Q_3)$ is indeed a constant. Thus, the coordinates $(\gamma^2 - 1)^{3/2} \equiv (p/m_0 c)^3$, $z \equiv Z(y)$, and L^3 are canonical in the present sense and are therefore eligible for use in (52), of which (4) is a special case. (Magnetospheric electric fields related to convection and corotation are implicitly neglected in the present work, as are day-night asymmetries in the magnetic field. This simplifying assumption is important for the validity of the above Q_i

as new variables, since it would be a mistake to adopt new variables that fail to remain constant around an adiabatic drift shell.)

The derivation of (4) from (52) is achieved by letting all of the transport coefficients except D_{zz} ($\equiv D_{22}$) vanish. In a description based on the uncanonical variables (E, x, L), this condition would be expressed by letting all of the transport coefficients except D_{xx} vanish. In this description, however, one must insert in (52) the Jacobian of the transformation from the canonical action variables (M, J, Φ) to the uncanonical variables (E, x, L) selected for their conceptual convenience (Haerendel, 1968; Schulz and Lanzerotti, 1974). One thereby obtains

$$\frac{\partial \bar{f}}{\partial t} + \frac{1}{G} \sum_{i=1}^{3} \frac{\partial}{\partial Q_i} \left[\left\langle \frac{dQ_i}{dt} \right\rangle G \bar{f} \right]$$

$$= \frac{1}{G} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial}{\partial Q_i} \left[D_{ij} G \frac{\partial \bar{f}}{\partial Q_j} \right] + \bar{S}, \qquad (61)$$

where $Q_1 = E$, $Q_2 = x$, $Q_3 = L$, and G is the Jacobian given by (57). One obtains (1) from (61) by letting all of the transport coefficients except D_{xx} vanish. This is the derivation described by Haerendel (1968). It is contingent upon the fact that all three of the adiabatic invariants (M, J, Φ) are canonical action variables (e.g., Schulz and Lanzerotti, 1974). Their conjugate phases (angle variables φ_i) are cyclic coordinates for the unperturbed Hamiltonian of charged-particle motion in the adiabatic guiding-center approximation.

An earlier derivation of (1) by MacDonald and Walt (1961) had been based on arguments of the type advanced in (48)-(51), namely that $xT(y)\,dx$ is a direct measure of phase-space volume at fixed E and L. Neither they nor Roberts (1969), however, chose to exploit the coordinate z as a natural variable for the construction of eigenfunctions. They chose instead to let $T(y)$ commute with $\partial/\partial x$ in (1).

SUMMARY

The major point of the present work has been to introduce the new canonical variable z, as defined by (3), in order to simplify the description of pitch-angle diffusion in a dipolar magnetic field. Various applications seem to follow quite naturally. For example, one can calculate eigenfunctions of the diffusion operator $(\partial/\partial z)[D_{zz}(\partial/\partial z)]$ by means of a quantum-mechanical perturbation theory, if not in closed form. The availability of such eigenfunctions enables one to calculate properly the temporal evolution of the phase-space density $\overline{f}$ from an arbitrary initial configuration toward an asymptotic steady state. It would surely be possible to identify further applications of the canonical diffusion coordinate z. Those noted above should suffice to establish the usefulness of the scheme. Numerical results illustrating implementation of the methods described above are given in an accompanying paper (Schulz and Boucher, 1981). Other applications are left (for now, at least) to the imagination of the reader.

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